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Exciton transport and orientationalglassification point in doped C60

Below 95 K, pristine fullerite C60 is in the state of orientational glass with all molecules performing rotational oscillatory motion. However not all the mutual orientations of pairs of molecules are energetically favorable. Saturation of fullerite with gases changes the situation. There were controversies [1,2] concerning what happens with the orientational glass state when C60 is stuffed with, for instance, with CO or NO.

Key words: glass transition point, excitons, X-ray analysis, luminescence.

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Перенос экситонов и приблизительная точка стеклования электронов в легированном C60

В настоящей работе мы использовали методы рентгеноструктурного анализа и люминесценции для изучения процесса интеркалирования C60 и водорода, азота, CO, а также последствий, вызванных интеркаляцией, воздействующей при высоких температурах до 350C и давлении 30 атм. Наши результаты показали, что механизм насыщения для H_2 значительно отличается от такового для N_2 и CO. Также наши эксперименты с люминесценцией с N_2 и CO в роли интеркалирующей добавки показали, что точка стеклования Tg смещается в область более низких температур, причем более явно в случае оксида углерода.

Ключевые слова: точка стеклования, экситоны, рентгеноструктурный анализ, люминесценция.

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Легирленген C60 электрондарының шынылаудың жуық нүктесі және экситондарды тасымалдау

Бұл жұмыста біз C60 және сутегінің, азоттың, CO интеркалировкалау процесін, сонымен қатар жоғары температурада 350C және қысымда 30 атм әсер ететін интеркаляцияның нәтижесін зерттеу үшін рентген құрылымдық талдау және люминисценция әдістерін пайдаландық. Біздің нәтижелеріміз H_2 үшін қанығу механизмі N_2 және CO қарағанда айтарлықтай ерекшеленетінін көрсетті. Сонымен қатар біздің интеркалировкалау қоспасы ретінде N_2 және CO қолданылған люминисценциямен тәжірибелеріміз Tg шынылау нүктесі көміртек оксиді қолданған жағдайға қарағанда айтарлықтай төмен температура аумағына ауысатынын көрсетті.

Түйін сөздер: шынылау нүктесі, экситондар, рентген құрылымды талдау, люминесценция.

Below 95 K, pristine fullerite C60 is in the state of orientational glass with all molecules performing rotational oscillatory motion. However not all the mutual orientations of pairs of molecules are energetically favorable. Saturation of fullerite with gases changes the situation. There were controversies [1,2] concerning what happens with the orientational glass state when C60 is stuffed with, for instance, with CO or NO. We used XRD and luminescence techniques to study the process of intercalation of C60 with hydrogen [3], nitrogen, and carbon monoxide as well as the consequences brought about by the intercalation, which was affected at elevated temperatures up to 350^0C (varying with the species being stuffed to avoid chemisorption) and at a pressure of 30 atm.

Our results [3] showed that the saturation mechanism for H2 differ essentially from those

for N_2 and CO. Equally, the consequences differ as much. Saturation with hydrogen proceeds in two stages, on the earlier of which octahedral voids are filled (at 250^0C it takes approximately 50 hours). After that double filling of octahedral voids begins, which has been clearly documented by the lattice parameter vs, time measurements. At that time point the integrated luminescence spectra as a function of temperature begin to change significantly. Unlike in pure C60, in which at the glassification point of Tg = 95 K the spectra start to decay with increasing T, the intensity stays virtually constant to a higher temperature the longer is the saturation time. we came to the following conclusions. First, the mechanism of luminescence suppression above Tg consists in the breaking of exchange paths of mobile excitons that produce the respective luminescence components, thereby stopping them and letting to get de-excited without emission. Second, Tg inevitably goes up until higher temperatures become capable of initiating molecular rotations.

In the case of N_2 or CO, the molecules are too big to occupy a single octahedral cavity with two intercalant particles. They can only expand slightly the cage thereby facilitating molecular rotations. Therefore, as show our luminescence experiments with these two intercalants the point Tg shifts to lower temperatures, more pronouncedly in the case of carbon monoxide.

References

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